

matrix elements of the bending co-ordinates for linear molecules, from which the g matrices of the bending coordinates of the UO_2 ion are calculated.

TABLE

Force constant	Description	Bent UO_2 ion (C_{2v}) ($\times 10^5$ dynes/cm.	Linear UO_2 ion ($D_{\infty h}$) ($\times 10^5$ dynes/cm.
f_d	O-U stretching	16.97	7.49
f_{dd}	Interaction between the two bonds	-0.77	-0.12
f_a	O-U-O bending	0.47	0.20
f_{da}	Interaction between the bond and angle	-2.31	0

The author is thankful to Dr. V. Santhamma for her help in the course of the calculations and to Dr. V. Ramakrishna Rao for his interest in the work.

REFERENCES

- Dacius, J. C., 1948, *J. Chem. Phys.*, **16**, 1025.
 Dieke, G. H. and Duncan, A. B. F., 1949, *Spectroscopic Properties of Uranium Compounds* (McGraw Hill publication).
 Feigle and Meister, 1951, *J. Chem. Phys.*, **19**, 982.
 Satyanarayana, B. S., 1942, *Proc. Ind. Acad. Sci.*, **15A**, 414.
 Wilson, E. B., 1939, *J. Chem. Phys.*, **7**, 1047.
 Wilson, E. B., 1941, *J. Chem. Phys.*, **9**, 76.

14

PHASE-TRANSITIONS IN $\text{Cu}[(\text{NH}_4)\text{SO}_4]_2 \cdot 6\text{H}_2\text{O}$

(Miss) GOURI BHOWMIK

DEPARTMENT OF MAGNETISM, INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE,
 JADAVPUR, CALCUTTA-32.

(Received, August 8, 1960)

Magnetic measurements showed (Bose, *et al.*, 1957 & 58) that the single crystals of many Tutton salts (composition $\cdot \text{M}(\text{AXY}_4)_2 \cdot 6\text{H}_2\text{O}$) lost their magnetic anisotropies in the range 65° – 120°C , probably due to a phase transition taking place which caused the single crystal to become polycrystalline. As a preliminary to studying the change in magnetic properties of the substance with change in structures, a study of the thermal dehydration of a typical case—that of $\text{Cu}[(\text{NH}_4)\text{SO}_4]_2 \cdot 6\text{H}_2\text{O}$, was undertaken which shows that there is a loss of 4 molecules of water at 67°C . The crystal structure of the dehydrated product was then

studied from X-ray powder photograph. It is found that the dehydrated product consists of the double salt $\text{Cu}[(\text{NH}_4)\text{SO}_4]_2 \cdot 2_2\text{H}_2\text{O}$. Application of Lipson's method (Lipson, 1949) shows that it has an orthorhombic unit cell having dimensions: $a = 14.84\text{\AA}$, $b = 12.52\text{\AA}$, $c = 10.69\text{\AA}$ containing 8 molecules per cell. Conditions of reflection suggest the possibility of assigning to the dihydrate either of the space-group $\text{P}_{mn}2_1$ or P_{mmm} .

Since direct X-ray data on $\text{Cu}[(\text{NH}_4)\text{SO}_4]_2 \cdot 6\text{H}_2\text{O}$ single crystal is lacking, we also undertook to study it and find that the hexahydrate which belongs to the space-group $\text{P}2_1/a$ and contains 2 molecules in the unit cell (Hofmann, 1931), has the following cell dimensions. $a = 9.27\text{\AA}$, $b = 12.50\text{\AA}$, $c = 6.33\text{\AA}$, $\beta = 106.5^\circ$.

It is interesting to note that the b axis in both the hexa- and dihydrate has the same length. It is, therefore, probable that the transition from the monoclinic to the orthorhombic system has taken place after merely a loss of 4 water molecules and a rearrangement of the molecules with reference to two vertical planes i.e., the transition is "topotactic" in nature.

Phase transition study for further dehydration and a more detailed study of structural changes by growing single crystals at high temperatures are under progress.

The author expresses her sincere thanks to Prof. A. Bose, D.Sc., F.N.I., for his kind interest and constant guidance and to Mr. S. Ray, M.Sc., for many helpful discussions during the progress of the work.

REFERENCES

- Bose, A., Mitra, S. C. and Dutta, S. K., 1957, *Proc. Roy. Soc., A* **239**, 165.
 Bose, A., Mitra, S. C. and Dutta, S. K., 1958, *Proc. Roy. Soc., A* **248**, 153
 Hofmann, W., 1931, *Zeits f. Krist.*, **78**, 279.
 Lipson, H., 1949, *Acta Cryst.*, **2**, 43

15

F-G MATRIX ELEMENTS FOR PYRAMIDAL XY_2Z MOLECULES

P. BABU RAO AND K. SREERAMAMURTY

PHYSICS DEPARTMENT, S. V. UNIVERSITY COLLEGE, TIRUPATI

(Received July 7, 1960)

Using Wilson's F-G matrix methods (1939, 1941), Pistorius (1959) obtained the elements for the planar XY_2Z type molecules employing the most general harmonic force field. These were recalculated by the authors (1960) and utilised to calculate the potential constants for certain specific cases. Venkateswarlu and Sundaram (1957) carried out a normal coordinate treatment for the pyramidal